

SUPPLEMENTAL DATA

for the paper

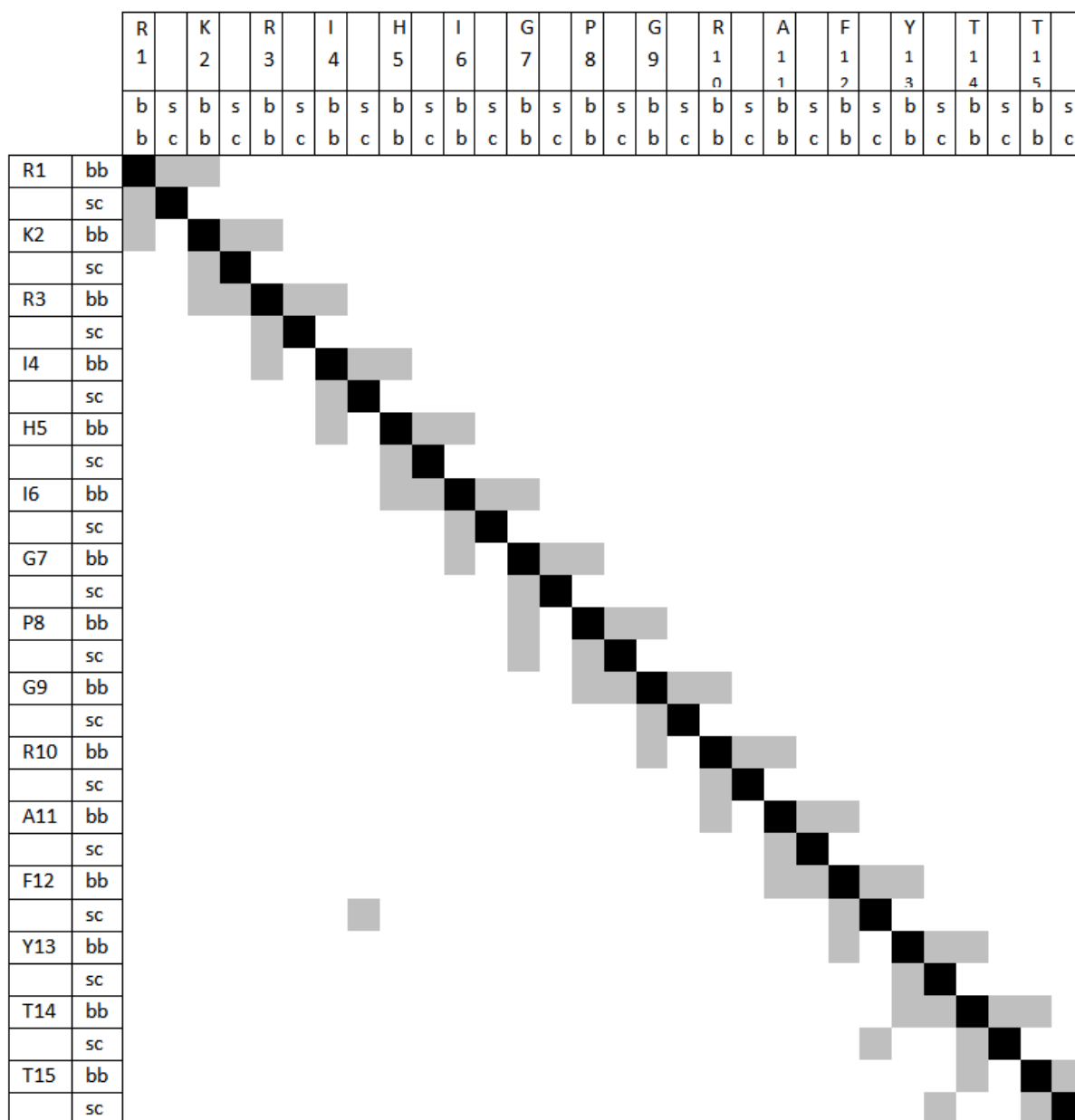
INTERACTION OF THE HIV-1 GP120 VIRAL PROTEIN V3 LOOP WITH BACTERIAL LIPOPOLYSACCHARIDE: A PATTERN RECOGNITION INHIBITION

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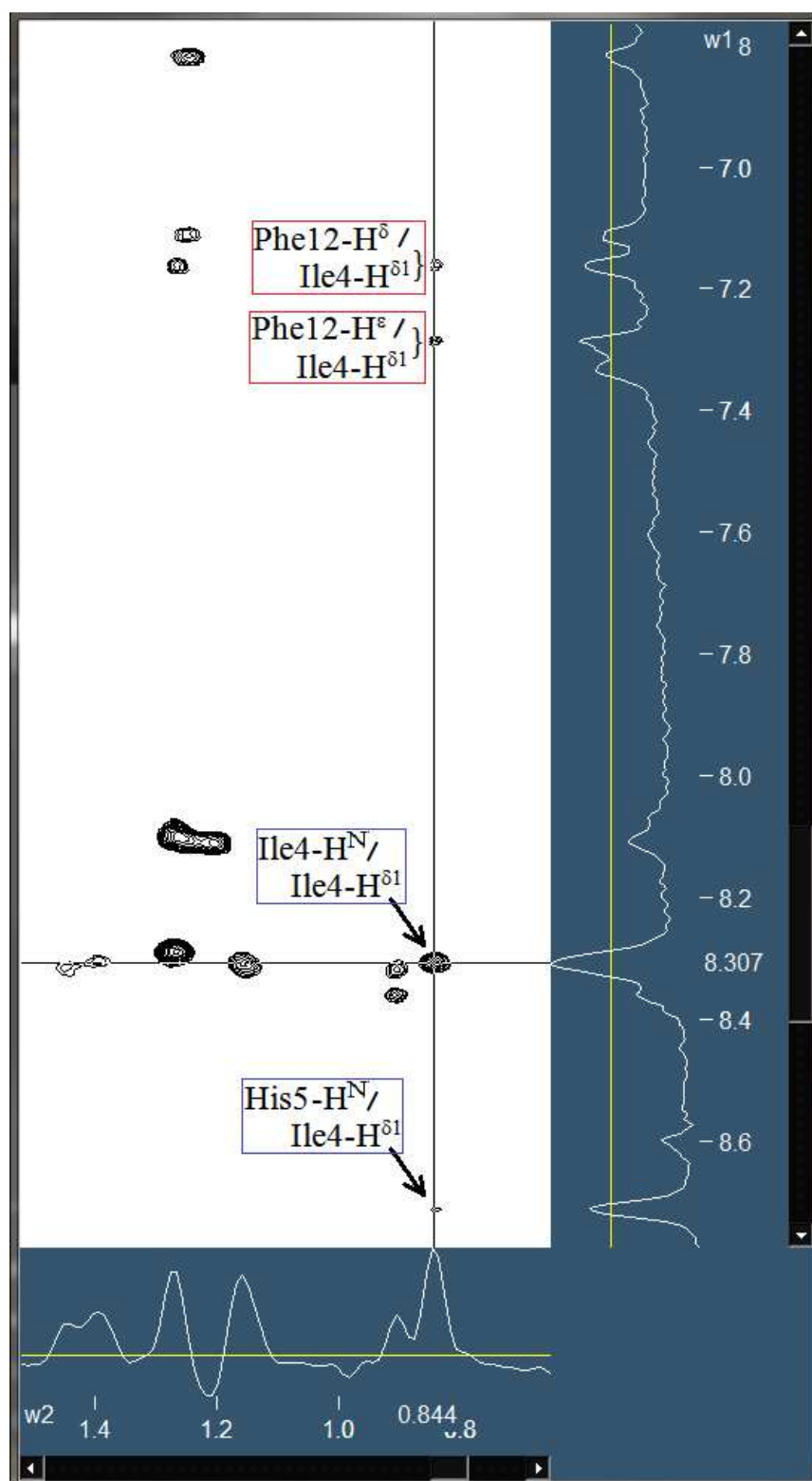
Running title: Interaction of the HIV-1 V3 loop with LPS

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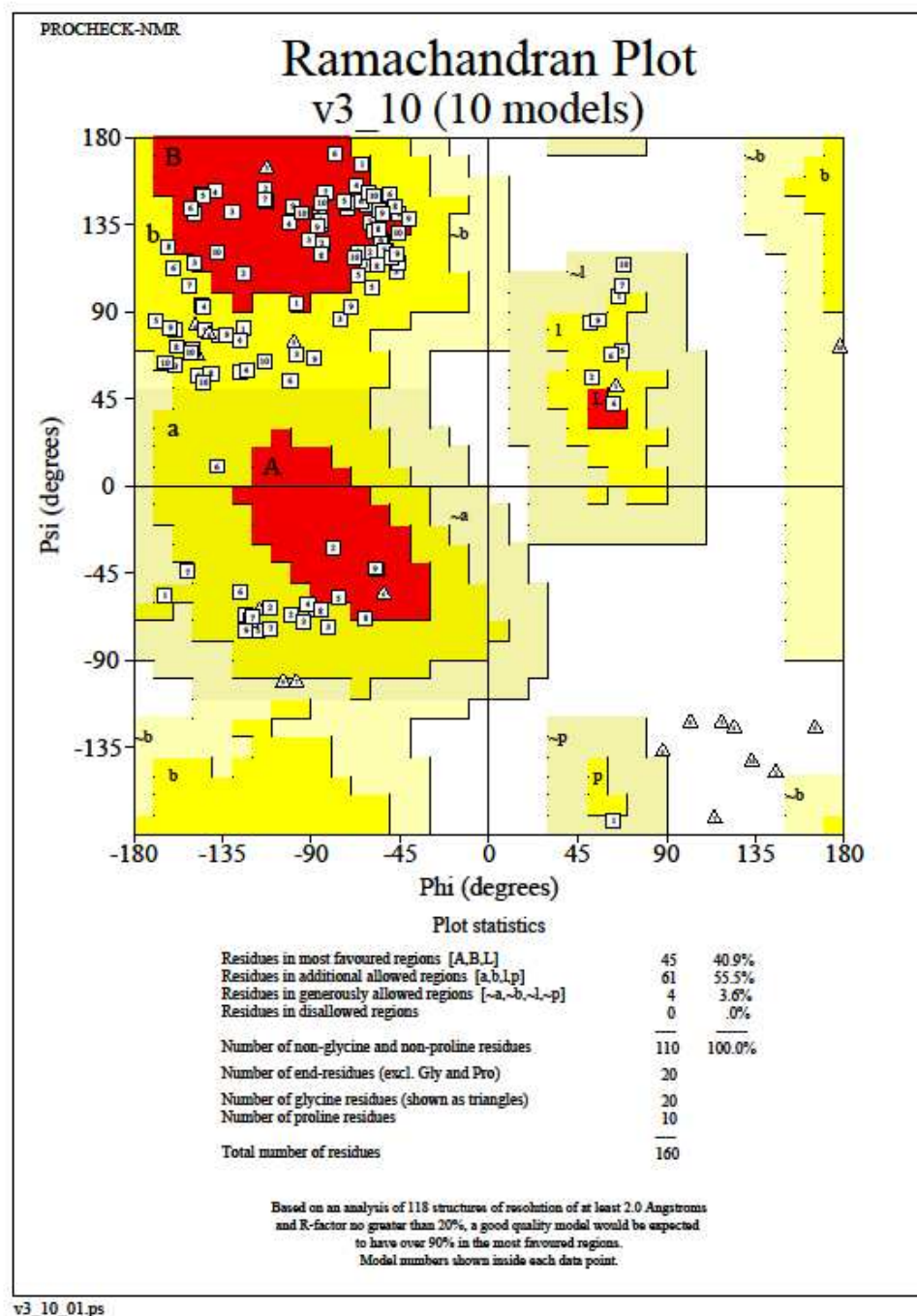
SUPPLEMENTAL FIGURES



Supplemental Figure S1. Patterns of NOE connectivities observed in (a) ROESY experiments (200 ms mixing time) of 2 mM V3 (above diagonal) and (b) NOESY experiments (80 ms mixing time) of 2 mM V3 in mixture with LPS at 10:1 w/w ratios (below diagonal). Any cross-peak observed between backbone (bb) and/or side-chains (sc) of the residues 1-15 (described with one-letter code) is depicted using a grey square; the diagonal is depicted with black squares.



Supplemental Figure S2. Detail from the NOESY spectrum (80 ms mixing time) of 2 mM V3 in mixture with LPS at 10:1 w/w ratio, showing the important long-range NOEs between residues 4 and 12 (in red). The Figure was produced using Sparky (1).



Supplemental Figure S3. Ramachandran plot of the ten best structures of V3 in complex with LPS.

SUPPLEMENTAL REFERENCE

1. T. D. Goddard and D. G. Kneller, SPARKY 3, University of California, San Francisco,
<http://www.cgl.ucsf.edu/home/sparky/>